Topical Report for Phase 1 Research

Numerical Investigation on the Maximum Entropy Eddington Factor Method in Transport Calculations

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This two-year DOE project is numerically investigating the possibility of using the Minerbo's Maximum Entropy Eddington Factor (MEEF) method in transport calculations. The MEEF method has been proposed as a low order approximation to transport theory. *A prior*, this method is very attractive because of its simplicity and ability of handling significant anisotropy of radiation flux and is expected to be much more accurate than other low order approximations and considerably faster than exact transport calculations. However, the feasibility and effectiveness of the method has not been established numerically. Furthermore, this method may suffer anomalous numerical instability. The goal of this research project is to numerically investigate the stability, validity and feasibility of the method and thus to decide whether it is practical to use it in real applications. Five specific tasks are proposed in the project: (1) Investigating the instability of the method; (2) Developing appropriate boundary conditions; (3) Comparing explicit and implicit treatments for the Eddington factors; (4) Comparing this method with the flux-limited diffusion approximations; and (5) Studying the accuracy and computational cost in general settings. Successful achievement of these objectives may establish the method as a useful algorithm in radiation-hydrodynamic simulations, reactor kinetics calculations, shielding calculations, and medical treatment applications, where accurate and fast computational algorithms are needed.

We have made satisfactory progress on the project and have achieved significant results during Phase 1. The effort in Phase 1 was focused on the feasibility and the virtue of the MEEF method. Several tasks in these aspects have been accomplished. The objectives and accomplishments of these tasks are described below.

a. Study the stability of the MEEF method

Stability is the first and most fundamental requirement for any numerical algorithm. The MEEF method has been observed to be unstable and yields anomalous results for some problems. Investigating the stability issue of the method is the most important ingredient of this project. The objectives of this task are to understand how the method works, identify reasons of instability, and find stable numerical schemes for the method, if existed. We accomplished the following on this task:

- Two reasons are identified to be responsible for the numerical instability under certain conditions;
- A theory is developed to predict when it becomes unstable when common iteration scheme is used; and
- One stable scheme was demonstrated to be appropriate for time-dependent transport calculations.

We presented these findings in *The 16th International Conference on Transport Theory*, May 10-15, 1999 at Atlanta, Georgia and submitted a scholarly paper on the work to the journal of *Transport theory and Statistical Physics*. A brief description of our work and accomplishments on this task is given below.

Several iteration schemes were used to solve the two Minerbo's MEEF moment equations. They consistently turned out to be conditionally stable. The stability of the method is problem dependent. To find out what causes the instability, Fourier stability analysis was performed to a class of problems. From the analysis, a spectral radius was derived, which predicts when the method is stable and when it is not. This analysis shows that for a conventional iteration scheme, the spectral radius changes monotonically from 0 to 2 with the scattering ratio decreasing from 1 to 0. For scattering ratio $c > 0.18$, the spectral radius is less than unity and thus makes the iteration process stable. For $c < 0.18$, the spectral radius is greater than unity, indicating that the numerical iteration is unstable. However, this instability does not seem to manifest itself as divergent growth, because the dominant eigenvalues at low frequencies are still within the unity circle on the complex plane and the unstable modes only occur at high frequencies. Such theoretical prediction on the stability agrees with numerical observations very well, both qualitatively and quantitatively. In addition, the stabilities of other Eddington factor closures in the literature are also analyzed. For instance, the Livermore-Pomraning closure is shown to have spectral radius that is never greater than unity. However, this closure is only marginally stable since its spectral radius is very close to one. Such predictions are also confirmed by numerical experiments. By analyzing the spectral radius for the Minerbo's closure, it is found the spectral radius becomes greater than one only when strong anisotropic radiation flux is involved, i.e., when the ratio of the two moments $\eta > 0.675$. Therefore it is only good to solve problems without too strong anisotropy of radiation field. This is the first reason for the numerical instability.

Further research reveals that there is another physical phenomenon that contributes to the numerical instability. The two moment equations with MEEF as a nonlinear closure have a critical point, at which the derivative of the radiation flux is undefined. Around the critical point, numerical solutions are very sensitive to small perturbations, even to round-off errors. Once a critical point exists in a problem, the solution of the two moment equations with the Minerbo's nonlinear closure cannot be obtained by common discrete mesh methods. Due to this critical point, some unphysical behaviors could be predicted by the MEEF method.

However, it is possible to somehow get around these numerical difficulties. Studies show that for time-dependent transport problems, upwind schemes for hyperbolic equations, like the approximate Riemann solver, can be used to predict smooth and stable solutions even near the critical point. We demonstrated the efficiency and accuracy of this approach and thus numerically proved that the MEEF method is really a better approximation than other low-order approximations available in the literature in the next task.

b. Compare the MEEF method with flux-limited diffusion approximations

The MEEF method is a low-order approximation as the flux-limited approximations existed in the literature. To make the method valuable and worthwhile, MEEF must be able to predict more accurate results than the flux-limited approximations, with no or little increase in computational cost. In this task, we compared these two approaches. The objective of this task is to draw convincing conclusions on the accuracy and computational cost of these two different, but closely related methods. This investigation would establish or de-establish the virtue of the MEEF method. We have performed several comparisons for this purpose. For one-dimensional time-dependent non-equilibrium radiation transfer problems, both the MEEF and flux-limited diffusive simulations were conducted and were compared to transport benchmarks. The results show that the MEEF method is able to predict very accurate results for radiative propagation and the MEEF method is significantly more accurate than all the flux-limited diffusions and other low-order

approximations. Furthermore, the MEEF equations were solved by an upwind scheme as an initial problem while the flux-limited diffusions must solve parabolic type boundary condition problems. Therefore, MEEF is in fact more cost effective in such circumstances, or at least at the same level of computational cost as other approximations. Based upon the comparisons we have done, we conclude:

- The Minerbo's Eddington factor method is consistently more accurate than classic and flux-limited diffusion theories; and
- The MEEF equations are not more costly to solve than flux-limited diffusion equations for time-dependent transport problems.

There are good reasons to believe that the first conclusion on accuracy holds for multi-group and/or multi-dimensional problems. However, it remains to be seen whether the second conclusion on computational cost holds or not in general geometry.

c. Compare the explicit and implicit treatments for the Eddington factors

This task concerns the efficiency of the method. For time-dependent problems, the Eddington factors can be treated in principle either explicitly or implicitly. Clearly, an explicit treatment is much faster than an implicit treatment, and thus is more appealing for practical use if there is no significant loss in accuracy. We have done some preliminary studies for this purpose. When conducting numerical simulations in the previous task, we tried both the explicit and implicit treatments for the Minerbo's Eddington factors. It seems that there are on significant differences between explicit and implicit results. However, no exclusive conclusion can be made at this moment, since only small time steps were used in these examples. More research needs to be done to draw a credible conclusion.